ASCEM FY10-FY15 Integrated Modeling Implementation Plan (WBS 1.1)

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EM Environmental Management

safety ❖ performance ❖ cleanup ❖ closure

Approval:

Dr. Paul Dixon, Los Alamos National Laboratory
Multi-Lab ASCEM Program Manager

9/20/10
Date

Dr. Juan Meza, Lawrence Berkeley National Laboratory
ASCEM Technical Integration Manager

9/20/10
Date

Dr. David Kosson, Vanderbilt University
Co-Project Lead Cementitious Barrier Partnership

10/20/10
Date

Heather Burns, Savannah River National Laboratory
Program Manager Cementitious Barrier Partnership

10/27/10
Date

Concurrence:

Jeff Griffin, Savannah River National Laboratory
ALD for Environmental Management

9/23/10
Date

Steven Schneider, EM-31
Office Director for Waste Processing

11/2/10
Date

Mark Williamson, EM-32
Program Manager ASCEM

11/1/2010
Date

Kurt Gerdes, EM-32
Office Director for Groundwater & Soil Remediation

9/24/10
Date

Yvette T. Collazo, EM-30
Director for Technology Innovation & Development

11/4/10
Date

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1. EXECUTIVE SUMMARY

The Advanced Simulation Capability for Environmental Management (ASCEM) program was initiated to support risk and cost reduction efforts across the U.S. Department of Energy's Office of Environmental Management (DOE-EM) and Technology Innovation and Development (OTID). ASCEM is a multi-institutional, collaborative effort between geoscientists, material scientists, and computational scientists from the Los Alamos, Lawrence Berkeley, Pacific Northwest, Oak Ridge, and Savannah River National Laboratories, with strong supporting technical assistance from Argonne, Idaho, and Lawrence Livermore National Laboratories. Current tasks associated with each of the participating laboratories are described in the *FY2010 Initiative Implementation Plan: Advanced Simulation Capability for Environmental Management (ASCEM),* while future tasks are described in this document.

This plan also serves as an update to the *FY2010 Initiative Implementation Plan*. It describes the multi-year (FY11 to FY15) effort and the synergistic relationships among the OTID offices' data collection and modeling efforts.

The ASCEM program supports DOE-EM OTID strategic initiatives by focusing efforts on the development of a state-of-the-art ***scientific tool and approach*** for understanding and predicting contaminant fate and transport in natural and engineered systems. The ASCEM program will specifically address the following critical EM program needs in order to reduce uncertainties and risks associated with DOE-EM's environmental cleanup and closure programs:

- The need to better understand and quantify the subsurface flow and contaminant transport behavior in complex geological systems to support the development and deployment of sustainable remediation technologies and strategies

- The long-term performance of engineered components, including cementitious materials in nuclear waste disposal facilities.

The ASCEM modeling initiative will develop an open-source, HPC modeling system for multiphase, multicomponent, multiscale subsurface flow and contaminant transport, and cementitious barrier and source-term degradation. The modeling tools will incorporate capabilities for predicting releases from various waste forms, identifying exposure pathways and performing dose calculations, and conducting systematic uncertainty quantification. ASCEM will demonstrate the modeling tools on selected sites and apply them in support of the next generation of performance assessments of nuclear waste disposal and decommissioning facilities across the EM complex.

In developing an integrated computer modeling system for multiphase, multicomponent, multiscale subsurface flow and contaminant transport, ASCEM will build upon national capabilities developed from decades of research and development (R&D) in subsurface geosciences, modeling and simulation, and environmental remediation. In addition, the integrated modeling tools will incorporate capabilities for predicting releases from various waste forms, identifying exposure pathways, performing risk and dose calculations, and conducting systematic uncertainty quantification. The ASCEM models will be demonstrated on selected sites and applied to support the next generation of performance and risk assessments for:

- Tank cleaning and area closure
- Long-term waste form performance assessment and analysis
- Sustainable groundwater and soil remediation solutions
- Decontamination and decommissioning (D&D) technology development and deployment
- Nuclear material disposition.

ASCEM will work in partnership with other related DOE modeling and risk reduction initiatives, including:

- DOE Office of Science's (SC) Subsurface Biogeochemical Research (SBR) Program

- DOE Office of Advanced Scientific Computing Research Office Scientific Discovery through Advanced Computing (SciDAC) program

- DOE Office of Health, Safety, and Security to ensure that the performance and risk tools are internally consistent with DOE regulatory practices

- DOE Office of Nuclear Energy high-performance computing (HPC) NEAMS modeling efforts

- DOE Office of Fossil Energy National Risk Assessment Program (NRAP) 2

- DOE National Nuclear Security Administration's Accelerated Strategic Computing (ASC) Initiative

- DOE-EM Low-Level Waste Disposal Facility Federal Review Group (LFRG) and the Performance Assessment (PA) Community of Practice (CoP) (PA CoP) by maintaining close ties with users via ASCEM's User Steering Committee

- Collaborations with the international community on HPC modeling**.**

This document summarizes how ASCEM will integrate and leverage the research and technology development efforts occurring in other programmatic areas within DOE-EM OTID and the other DOE offices to produce a transformational, graded, and iterative modeling and simulation approach to meet EM's long-term risk and performance modeling needs. This will also address Assistant Secretary of DOE-EM visionary request to the DOE-EM staff to develop technologies dependent upon transformational advances in science and engineering in both the short- and long-term to solve the remaining remediation challenges, which are more complex than those DOE has dealt with in the past.

2. THE ASCEM INTEGRATED MODELING EFFORT

OTID's mission is to develop technologies that advance the safe and timely cleanup of legacy wastes and facilities from defense nuclear applications. This is the largest cleanup program in the world [1]. Although EM has made great progress toward this goal during the past twenty years, the remaining clean-up challenges are far more complex than those previously addressed. The role of the ASCEM initiative is to develop a transformational modeling approach and toolset to help EM better meet these challenges through improving its long-term risk and performance modeling capabilities and by characterizing and reducing the uncertainty associated with the resulting predictions.

To support the EM OTID strategic initiative, ASCEM will focus on understanding and improving the predictive modeling capabilities within EM in the areas of:

- Subsurface flow and contaminant transport behavior in complex geological systems
- The long-term performance of engineered components and barriers, including cementitious materials in nuclear waste disposal facilities.

The DOE Offices of Science, Nuclear Energy, and Fossil Energy have made significant investments in developing advanced, high performance computing models for evaluating groundwater flow and transport, source term degradation and release, and mechanical degradation of structures and barriers. ASCEM will leverage these investments. In doing so, ASCEM will improve the timeliness and cost effectiveness of its modeling approach and toolset, which will not only benefit DOE-EM, but the greater DOE community as well (e.g., in the areas of geologic sequestration of carbon and high level waste repository performance).

The ASCEM model will initially provide additional technical underpinning to the existing risk and performance assessments currently being developed and defended across the EM complex. The need for this support has been determined through interviews with the EM site end-users [2]. End-users will also be critical in developing the ASCEM modeling tools requirements and design documents.

2.1 Introduction to Program Needs

In response to a congressional request for an R&D roadmap to support EM cleanup efforts, DOE-EM identified key engineering and technology gaps for EM programs.[1] In a review of the roadmap, the National Research Council (NRC) of the National Academies provided advice to DOE-EM for addressing principal science and technology gaps.[2] Table 1 shows the principal technology gaps

[1] DOE-EM Engineering and Technology Roadmap: Reducing Technical Uncertainty and Risk in the EM Program, March 2008,
[2] National Research Council Committee on Development and Implementation of a Cleanup Technology Roadmap, Advice on the Department of Energy's Cleanup Technology Roadmap: Bridges and Gaps, 2009

identified by DOE in their groundwater and soil remediation program and NRC's ranking of their R&D priority.

Table 1. *Principal Science and Technology Gaps and Their R&D Priorities.*

GS#	Gap	Priority
GS-1	Contaminant behavior in the subsurface is poorly understood.	High
GS-2	Site and contaminant source characteristics may limit the usefulness of baseline subsurface remediation technologies.	Medium
GS-3	Long-term performance of trench caps, liners, and reactive barriers cannot be assessed with current knowledge.	Medium
GS-4	Long-term ability of cementitious materials to isolate wastes is not demonstrated.	High

To address these gaps, NRC provided a series of recommendations, one of which focused on the development and use of advanced computational models. NRC advised that these modeling tools should:

- Incorporate understanding of site geohydrology and contaminant geochemistry, with the goal of improving the currently insufficient scientific knowledge base (GS-1)
- Include robust models of caps/covers, barriers, and cementitious materials/ waste forms (GS-3)
- Incorporate appropriate uncertainty (GS-1, GS-2, GS-3, and GS-4)
- Account for natural and anthropogenic spatial and temporal changes, together with field data to calibrate these models (GS-3 and GS-4)
- Develop predictive capabilities to understand contaminant behavior and to support developing and implementing effective and sustainable remediation approaches (needs previously indentified in internal workshops and reviews [3, 4]).

In response to the NAS and internal DOE review recommendations, and to address key challenge areas including GS-1, GS-3 and GS-4, DOE-EM has launched the ASCEM initiative along with other complementary and synergistic initiatives, including collaborations with the DOE Offices of Fossil Energy (DOE-FE), Nuclear Energy (DOE-NE), and SC.

3. INTEGRATED MODELING VISION - ASCEM

Bridging the gap between basic science and "needs-driven" applied research is a universal challenge for all areas of technology development. This is particularly true for DOE-EM because the organization faces cleanup and waste management problems of increasing complexity. The ASCEM modeling initiative will enable DOE-EM to deal with these complex problems by providing the technical underpinnings needed to ensure that decisions are based on the best available scientific knowledge.

ASCEM is a state-of-the-art scientific tool and approach for integrating data and scientific understanding to enable prediction of contaminant fate and transport in natural and engineered systems. The initiative supports the reduction of uncertainties and risks associated with DOE-EM's environmental cleanup and closure programs by better understanding and quantifying the subsurface flow and contaminant transport behavior in complex geological systems. A second aspect addresses the long-term performance of engineered components, including cementitious materials in nuclear waste disposal facilities.

The ASCEM modeling initiative will develop an open-source, HPC modeling system for multiphase, multicomponent, multiscale subsurface flow and contaminant transport, and cementitious barrier and source-term degradation. The modeling tools will incorporate capabilities for predicting releases from various waste forms, identifying exposure pathways and performing dose calculations, and conducting systematic uncertainty quantification. ASCEM will demonstrate the modeling tools on selected sites and apply them in support of the next generation of performance assessments of nuclear waste disposal and decommissioning facilities across the EM complex.

A major ASCEM goal is to provide a community code for DOE-EM and the greater scientific and engineering communities. To that end, the ASCEM HPC modeling tools will be developed using an open source model, with involvement from the DOE-SC community. This method will allow ASCEM to leverage the considerable scientific investment that has already been made both within and outside of DOE-EM in the areas of subsurface geosciences, modeling and simulation, and environmental remediation.

For example, within DOE-EM collaborations exist between the EM-31 Cementitious Barriers Partnership (CBP)[3] and EM-32 field demonstration and Landfill Partnership[4] efforts. *Figure 1* illustrates the programmatic interrelationships:

- The CBP characterizes the structural, hydraulic, and chemical performance of cement barriers, including both containment structures and waste forms. This knowledge enables improved evaluations and system designs.

- The DOE Landfill Partnership addresses technological issues related to on-site disposal facilities (labeled "landfills" in *Figure 1*) in the DOE complex that receive low-level wastes and mixed wastes from decommissioning projects. These issues include design, operations, and prediction of long-term performance.

- EM-32 provides the capabilities necessary to understand the source zone characteristics, release rates, migration velocities, and spatial distribution of subsurface contaminant plumes.

[3] A brief summary of CBP is provided as Appendix C.
[4] A brief summary of the Landfills Partnership is provided as Appendix B

Through integrating these efforts, ASCEM will facilitate development of more accurate site models, allow for predictive simulation of proposed remediation methods, and prevent implementation of overly conservative and unnecessarily expensive remediation strategies. Wherever appropriate, ASCEM will use and build upon results and models developed through its associated DOE initiatives.

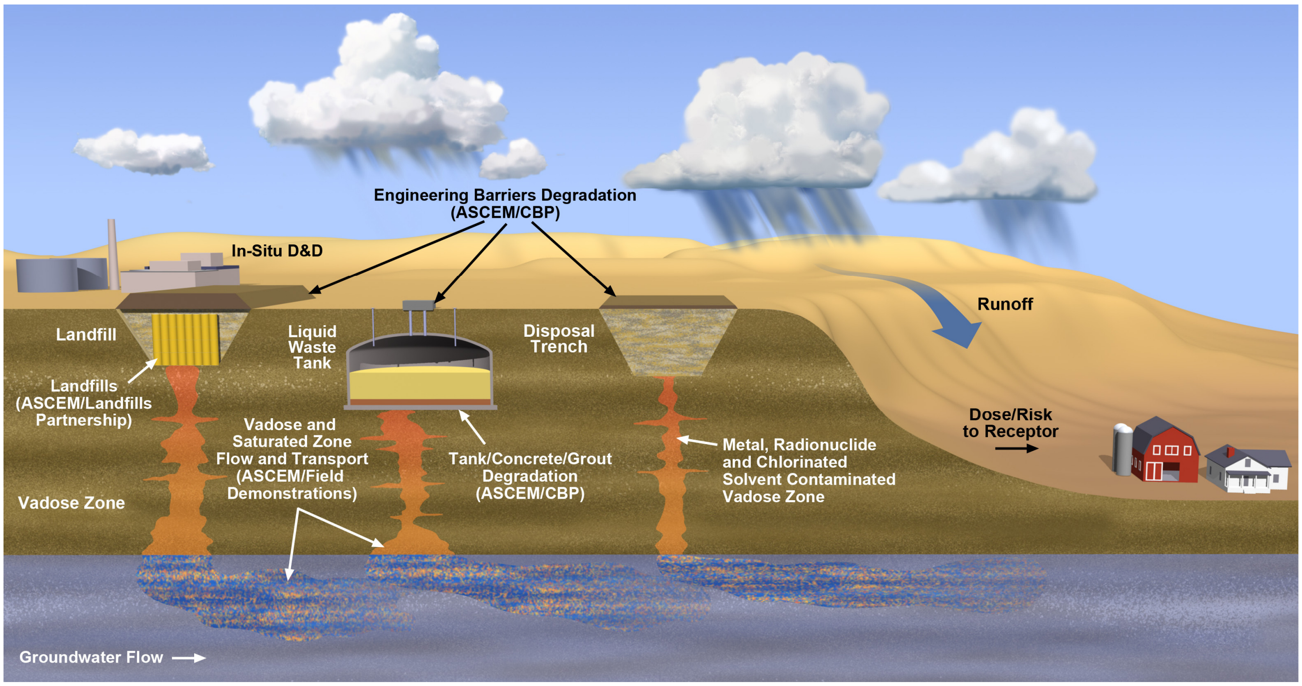

Figure 1. Typical environmental processes considered in ASCEM integrated modeling initiative.

Within DOE Offices of Science, Nuclear Energy, and Fossil Energy there are many efforts in the development of advanced HPC capabilities, as well as scientific investigations of groundwater flow and transport, source term degradation and release, and mechanical degradation of structures and barriers. By leveraging these investments, ASCEM will develop a toolset for use not only within DOE-EM, but also by the greater DOE community in the areas of geologic carbon sequestration and high-level waste repository performance. ASCEM has already established ties with each of these DOE Offices (as outlined in section 7), and will strengthen them through close interactions during the development cycle and during investigations of new research areas.

3.1. ASCEM Technical Organization

The ASCEM project is organized into three technical thrust areas: the Multi-Process High Performance Computing Simulator (HPC Simulator), which constitutes the computational engine; the Platform and Integrated Toolsets, which provide the user interfaces; and Site Applications (see *Figure 2*). Detailed descriptions of the three thrust areas are contained in the FY2010 Implementation Plan.

The Site Applications thrust area provides the main link between ASCEM and the EM community's modeling and regulatory needs; it is vital to ensuring that ASCEM HPC modeling capabilities are widely accepted across the EM Complex. Because engaging the user community will be particularly important in the early stages of the ASCEM development, the Site Applications thrust area incorporates a "user interface" task focused on establishing contact with end users, soliciting their input about ASCEM development plans, and conveying the feedback to members of the HPC and Platform Thrust areas responsible for the tool and code development.

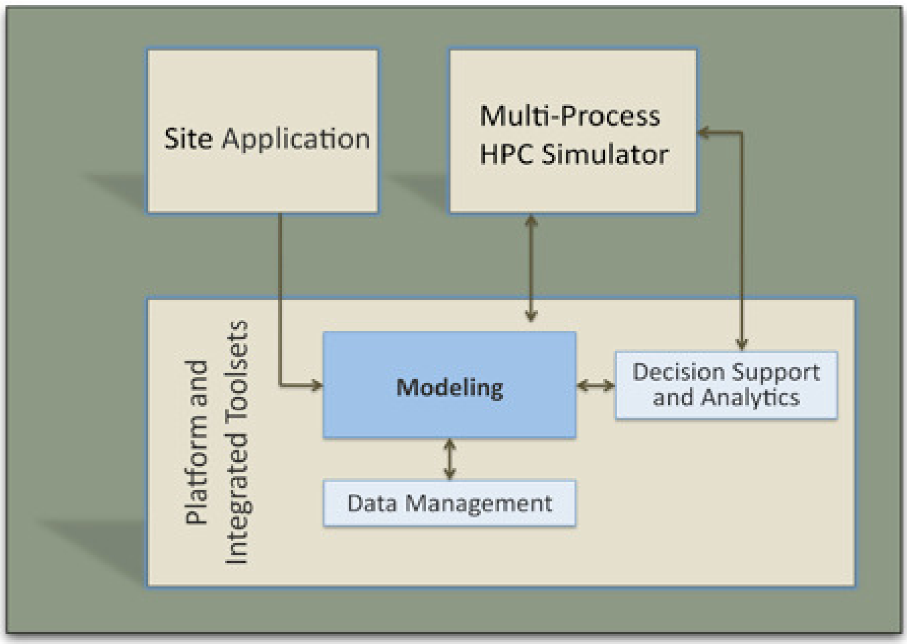

Figure 2. The 3 technical thrust areas of ASCEM: Multi-Process HPC Simulator, Platform and Integrated Toolset, and Site Applications.

The Platform and Integrated Toolset thrust will provide a standardized user interface enabling end users to create inputs, analyze outputs, and manage data associated with running simulations and performance and risk assessments. Under this thrust area, ASCEM will use a modular (or "interoperable") approach to code development, facilitating iterative and graded modeling systems that allow end-user customization for specific applications without the need for specialized computational or code development expertise. This will be accomplished by defining rigorous programming "interfaces" for each module (where an interface defines access to a module while hiding the details of its implementation). By using a common base platform available to all, this interoperable approach will support cooperation among numerous modeling groups with different methodologies and applications. This methodology has been quite successful in the past and is broadly used in similar advanced software engineering approaches, for example, within the SciDAC program and the DOE National Nuclear Security Administration (NNSA) ASC program. This modular approach will also be used to develop new, correct, and complete process models that are imperative for successfully implementing performance and risk assessment approaches.

The third thrust area, the Multi-Process High Performance Computing Simulator, will provide the simulation capabilities necessary for the modeling of EM sites. The HPC Simulator will provide a flexible and extensible computational engine to simulate the coupled processes and flow scenarios described by the conceptual models developed using the ASCEM Platform. The graded and iterative approach to assessments naturally generates a suite of conceptual models that span a range of process complexity, potentially coupling hydrological, biogeochemical, geomechanical, and thermal processes. To enable this approach, ASCEM will take advantage of emerging petascale computers that handle hundreds of thousands of simultaneous process streams of information. Their use will facilitate improved uncertainty quantification and, when necessary, the use of more complex models in lieu of simplifying assumptions. These HPC-capable tools will be available on platforms from clusters to desktop computers. While there is a clear recognition that many problems will not require the highest end computing capabilities, computer architectures on today's supercomputers will be used on desktop computers in the near future (5-7 years). By developing the ASCEM modeling tools for HPC platforms, the community code will be well positioned to run on future desktops.

Finally, the ASCEM modeling capability will be made available to EM site users through training and technology transfer. It will also be made available to the greater scientific community for use in subsurface and risk analysis research and for creating additional modules incorporating scientific advances and new research areas.

3.2. The ASCEM Software Lifecycle Model

ASCEM code development will occur in three overlapping phases over the next four years, as shown in *Figure 3*. Each phase continues as capabilities are added based on EM's regulatory needs.

ASCEM code development will begin at the R&D phase. During this phase, the code requirements and design will be defined and developed using standard software quality assurance practices, and the code capabilities will be tested and validated. Once tested and validated, the ASCEM R&D code will move into the Applied (Community Code) phase for use at the various EM sites for non-regulatory work. The Community code is the open source version that can be used by entities (DOE-FE, DOE-SC, and DOE-NE) outside of EM as a shared community model. Finally, at strategic times the Community Code will be brought under full NQA-1 quality assurance (QA) requirements and made available to EM for use as their standardized risk and performance assessment code. Thus, at any future time, there may be three versions of the ASCEM code co-existing between the three lifecycle phases. Phased code development allows only the full regulatory parts of the ASCEM code to undergo the costly NQA-1 requirements, thus allowing development and use of a viable community code without this overhead.

The software QA program as described in the Project Quality Assurance Plan for ASCEM is based on the NQA-1 standard (2004 with the 2005 and 2007 Addenda) using a graded approach to the project efforts (based on Subpart 4.2). As the ASCEM code moves from R&D, to applied research, and finally to the regulatory (full implementation) phase, the importance and specificity of the QA requirements increase. As the code is developed in each phase, it will be tested and validated using appropriate software QA practices and configuration management practices.

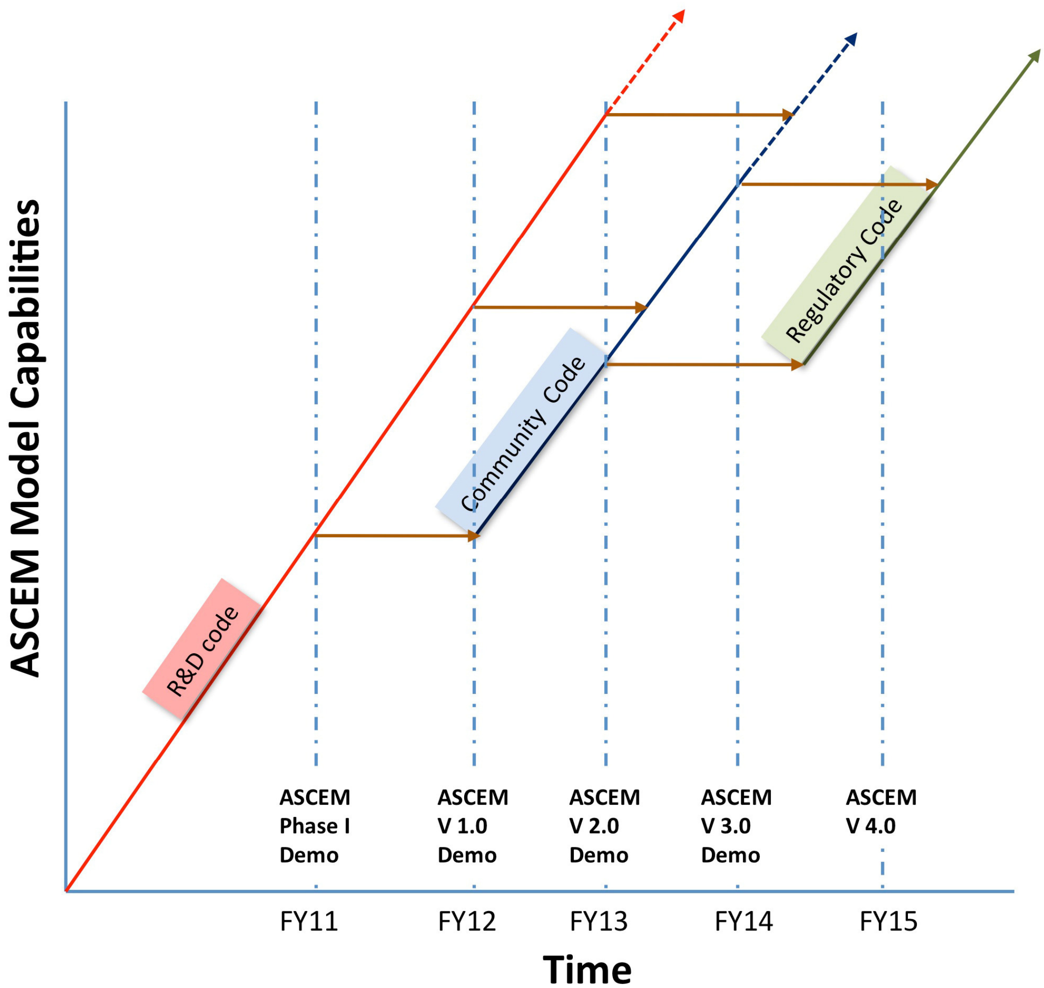

Figure 3. ASCEM software lifecycle illustration: R&D code evolves into Community Code (Applied phase), which is then used as the basis for the Regulatory Code.

4. PROGRAM REQUIREMENTS

The success of the integrated OTID ASCEM initiative requires that policy, institutional, and/or budget requirements be addressed as part of project planning and execution. Specific requirements to be addressed are:

- Coordination with site performance and risk assessment characterization and scientific investigations to generate data required for ASCEM validation and verification
- Coordination and collaboration with site contractors and regulators to assure that remediation contractors will use ASCEM products to meet regulatory requirements

- Assurance that project activities and deliverables can be completed soon enough to impact remediation and site closure decisions

- Potential need for additional field activities in support of Area Closure to generate unique site characterization data to support model validation and verification activities

- Need to maintain funding profiles for ASCEM and synergistic and supporting EM initiatives (these funds need to be available at the start of each fiscal year to accomplish the programs goals in the aggressive time frames described in this implementation plan)

- Need to maintain expertise and resources necessary to address EM's long-term needs (i.e., field test facilities and information archives) to develop detailed conceptual understanding and site models to guide remediation actions and support DOE's long-term stewardship planning.

5. PROGRAMMATIC AREAS

ASCEM is poised to integrate many programs across the DOE Complex, academia, and industry in efforts ranging from modeling, laboratory R&D, and meeting regulatory requirements. However, the primary EM-30 integration efforts are between the EM-32 Groundwater and Soil Remediation Program (GW&S) and the CBP program sponsored by EM-31. The goals of these two programs are described briefly below.

5.1. Groundwater and Soil Remediation Program: Subsurface Processes, Treatment, and Monitoring

A major component of DOE's environmental management mission is the cleanup of groundwater, soils, and sediments in highly diverse environments contaminated with radionuclides, metals, organics, and in some cases, complex mixtures.

Although EM has made significant progress in its restoration efforts at sites such as Fernald and Rocky Flats, many of the remaining challenges are the most complex ever encountered by the subsurface science community, particularly at the larger sites such as the Savannah River Site (SRS), the Oak Ridge Reservation (ORR), and the Hanford Site.

- SRS, located in south-central South Carolina, has an extensive groundwater plume containing radionuclides and nitrates at concentrations that exceed maximum contaminant levels. Additionally, the leakage of low-level radioactive waste, mixed waste, and intermediate-level radioactive waste disposed of in burial grounds in the central part of SRS has resulted in groundwater plumes that contain various organic solvents, heavy metals, and radionuclides.

- ORR, located in eastern Tennessee, has extensive contamination, including mercury contamination of soils, groundwater, surface water, and biota. Additionally, significant amounts of other contaminants released into the environment have created large groundwater plumes that discharge into nearby creeks and water bodies.

- The Hanford Site, located in southeastern Washington State, has subsurface environments that consist of complex stratified layers of unconsolidated sediments that may interact with surface waters of the bordering Columbia River and groundwater at depths that are hundreds of feet thick. These environments contain groundwater and sediment contaminated with numerous contaminant plumes containing radionuclides, inorganic compounds, and organics.

DOE-EM developed the Engineering and Technology Roadmap to help meet the subsurface challenges described above. This roadmap identified four strategic groundwater and soil remediation initiatives:

- Improved Sampling and Characterization
- Advanced Predictive Capabilities
- Enhanced Remediation Methods
- Enhanced Long-term Performance Evaluation and Monitoring.

These initiatives are the basis of GW&S. To efficiently complete them, the program was organized into strategic action areas addressing specific components of a systems-based approach to remediation and closure, with ASCEM as the integration framework supporting them:

1) Attenuation-based remedies for metals and radionuclides
2) Advanced remediation methods for metals and radionuclides in the vadose zone (scientific and technical basis for *in situ* treatment systems for metals and radionuclides)
3) Remediation of chlorinated solvents in the vadose zone and groundwater
4) Mercury characterization and remediation
5) ASCEM.

Drawing on ASCEM to meet the research challenges addressed in the action areas will provide the technical foundation for a systems-based approach to cleaning up the remaining subsurface contamination (*Figure 4*). Each action area involves controlling processes, characterizing heterogeneities, providing for subsurface access and delivery, monitoring, and modeling, and each "piece of the puzzle" interconnects with the others to enable development and implementation of holistic remediation strategies based on a scientific understanding of the subsurface environment.

Predictive models are the primary tool for forecasting evolving subsurface processes and scenarios to assess and optimize the potential efficacy of remediation strategies. Such models are the framework for knowledge integration. ASCEM provides this framework through integrating basic science and applied research obtained from the different aspects of subsurface science—biology, geochemistry, and hydrology—into a form that will provide the defense-in-depth needed to address remaining subsurface challenges. ASCEM will enable more accurate predictions of contaminant fate and transport, as well as the design and implementation of remediation approaches and performance monitoring approaches for the GW&S program. The incorporation of data obtained at the three integrated field research sites (geohydrology characterization, design and implementation of remediation and monitoring systems, and investments leveraged from other relevant organizations [e.g., SBR Program]) is expected to facilitate the transition of scientific results into applied solutions.

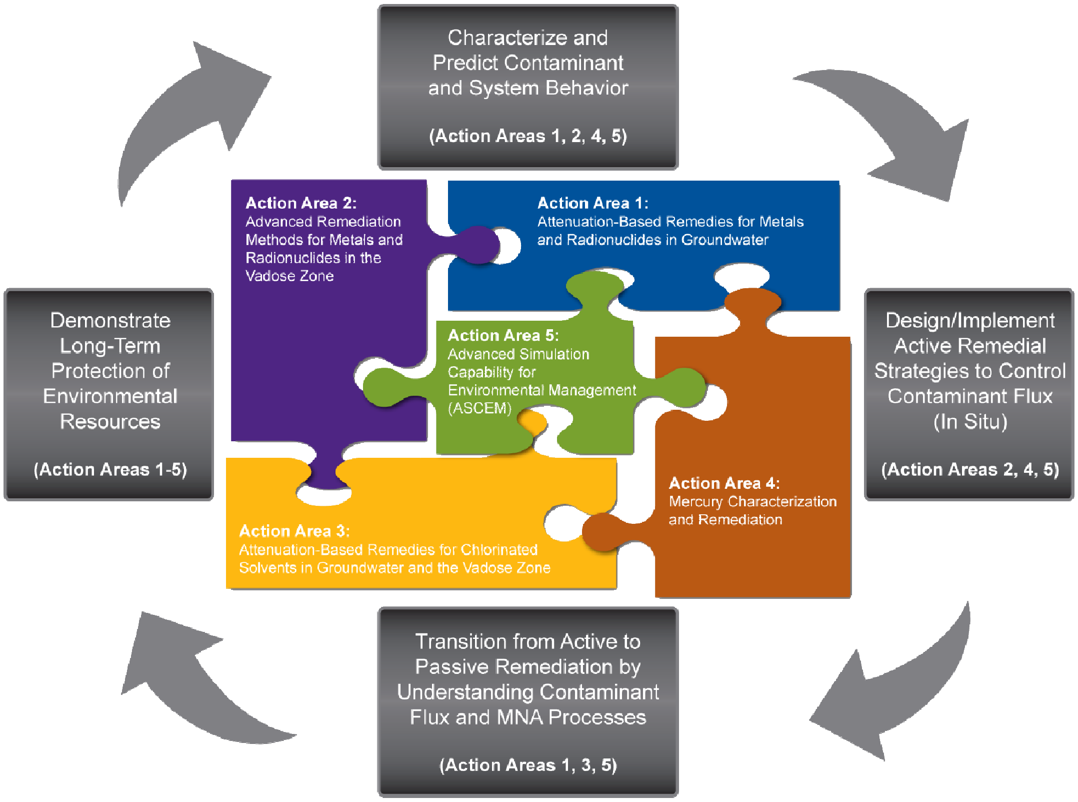

Figure 4. Groundwater and soil remediation program strategic action areas.

The integrated strategy being conducted at the three field research sites is discussed in Appendix D.

5.2. Long-Term Performance of Engineered Components

The major integration thrusts supported by EM are 1) the long-term performance of engineered components and 2) the GW&S program (see *Figure 7*). The long-term performance of the engineered components will be informed by CBP and the Landfill Partnership. To enable improved risk-informed, performance-based decision making, the CBP is developing a credible set of simulation and modeling tools to predict the structural, hydraulic, and chemical performance of cement barriers used in nuclear applications over extended time frames. Applicable barriers include cementitious and other related waste forms, high-level waste tank closures, D&D of nuclear material processing facilities, *in situ* grouting of soil, vadose zone contamination, and life extensions of nuclear facilities. The DOE Landfill Partnership will conduct the applied research and facilitate the technical dialogue needed to build confidence in technologies used for on-site disposal facilities, the methodology used to design and assess the facilities, and the systems used to monitor long-term performance. The modeling efforts in the CBP, Landfill Partnership, and GW&S action areas will be fully integrated with the ASCEM program.

Detailed information on CBP and the Landfill Partnership can be found in Appendices B and C, respectively.

5.3. ASCEM - Integration of Programmatic Areas

Emergent phenomena cause complex environmental systems to behave in unpredictable ways—ways that cannot be anticipated from an understanding of the individual components. These behaviors impact the approach to R&D integration. The scientific and engineering challenges inherent in remediating such complex systems (e.g., *Figure 1*), illustrate the value of HPC in more accurately modeling these complex and dynamic environments.

ASCEM's computational predictions will enhance understanding of the temporal and spatial controls of systems-based performance for engineered barriers, wasteforms, subsurface enhanced and natural attenuation mechanisms, and the evolution of controlling processes (e.g., hydrogeologic and biogeochemical conditions). The ASCEM modeling platform will fully integrate EM site, field, and laboratory data, enabling system model simulations that will reduce uncertainty in long-term performance predictions. ASCEM's ability to describe and integrate key processes using computer simulations will provide more robust quantitative support for environmental decisions.

This approach provides a strategic framework to integrate and translate the scientific and engineering underpinnings on which environmental decisions are based, allowing DOE-EM to:

- Provide scientifically defensible predictions of contaminant behavior over spatial and temporal scales relevant to DOE EM's clean up/closure efforts
- Develop and implement sustainable remediation strategies
- Provide a consistent approach to performance assessment that can guide remediation treatments, site closure, and long-term waste management decisions across the EM complex
- Design engineered solutions (i.e., engineered barriers and landfills) capable of altering the environment in ways that stabilize and shrink contaminant plumes.

6. PROJECT ORGANIZATION AND MANAGEMENT MODEL

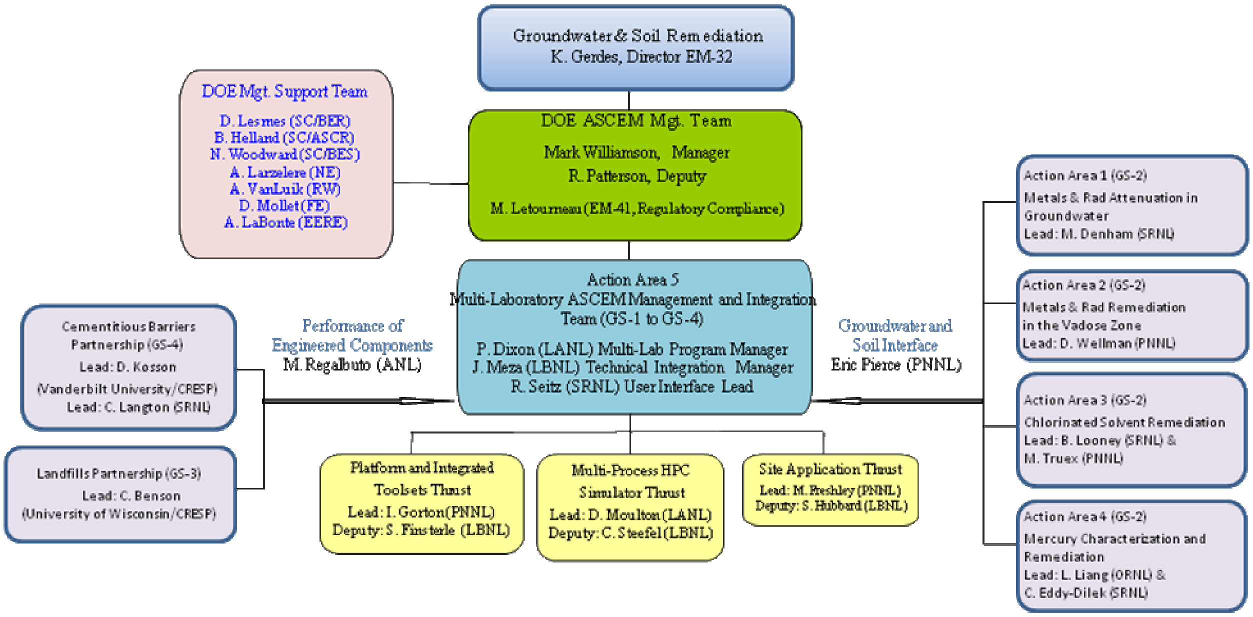

Figure 5. ASCEM project organization and interrelationship chart.

Figure 5 illustrates the organizational breakdown structure (OBS) for the ASCEM Program. The modeling efforts in CBP, Landfill Partnership, and GW&S areas will be fully integrated with the ASCEM modeling program. The key integration interfaces and current leadership of these areas are also illustrated in *Figure 5*. Also shown are these modeling efforts' ties to the NAS groundwater and soil remediation recommendations (i.e., GS-1 to GS-4).

7. PARTNERSHIP WITH OTHER DOE OFFICES AND INTERNATIONAL ORGANIZATIONS

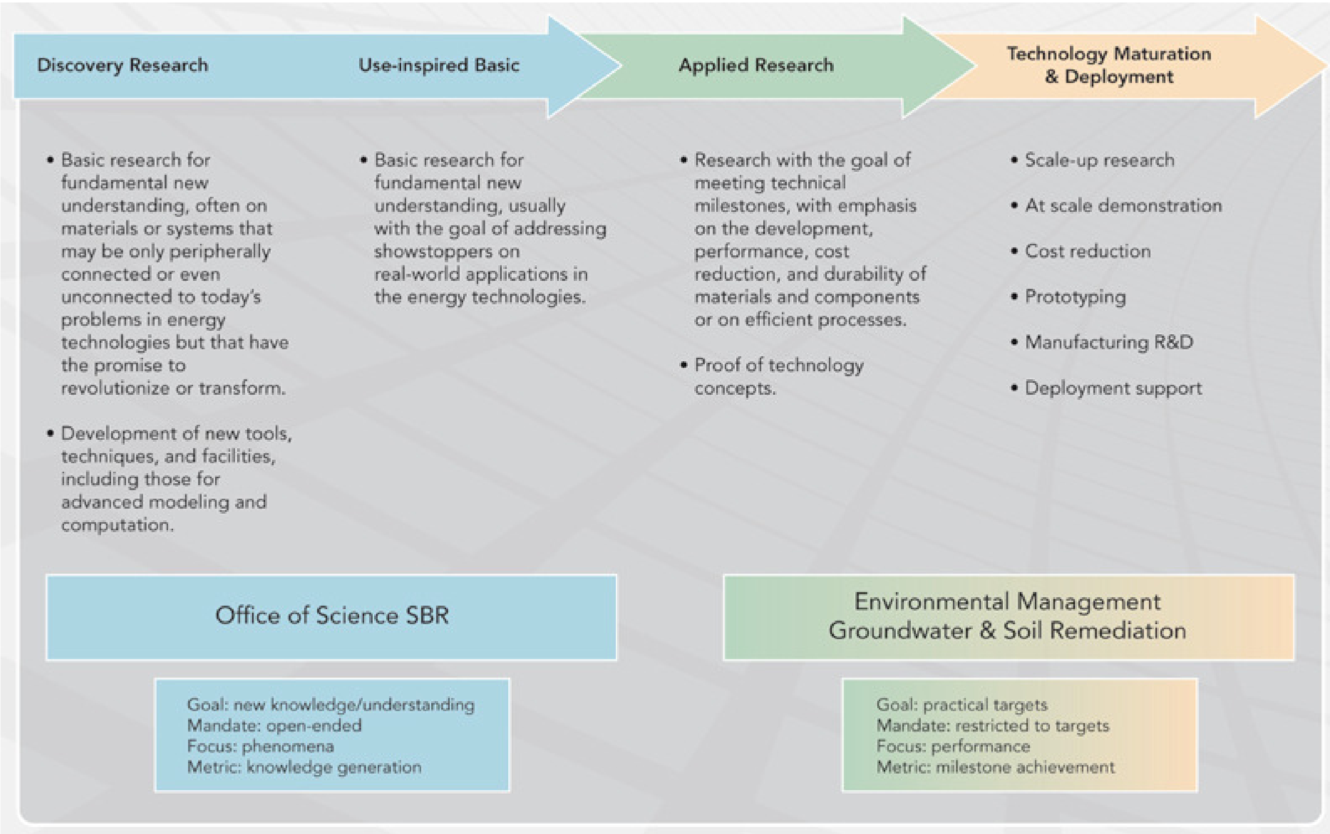

Figure 6. Example of the interface between basic science (SC) and applied research (EM).

ASCEM will leverage the efforts of and integrate with other DOE science and computing initiatives. *Figure 6* illustrates concepts associated with the maturation of basic research into production-ready engineering solutions, along with SC and EM domains within the process. To facilitate such maturation, the following integration efforts are currently under way:

- Integration with the SBR Program in modeling and HPC, geohydrology, geochemistry, geophysics, microbiology, and remediation. ASCEM will also use the data-rich SFA and information generated as part of SBR's integrated field research challenges to allow testing and demonstration of the ASCEM toolset. In addition, the SBR SciDAC program's modeling efforts will be leveraged and integrated to quickly advance ASCEM's modeling capabilities in the areas of HPC software infrastructure development, numerical libraries, data management, and visualization efforts.

- Integration with DOE's Office of Health, Safety, and Security to make sure that the performance and risk tools are internally consistent with DOE regulatory practices. The ASCEM team is also working closely with former Yucca Mountain PA specialists to leverage expertise to support the next-generation EM PA toolset.

- Integration with the DOE-NE Nuclear Energy Advanced Modeling and Simulation efforts in source-term and waste-form modeling, and the next-generation, high-level waste, performance assessment models being developed under the NE Used Fuel Disposition campaign. There is great potential synergy between the NE repository performance assessments code development and ASCEM that should be tapped, perhaps through a joint NE/EM performance assessment modeling workshop.

- In addition, as the DOE-FE begins its NRAP on geologic sequestration of CO_2, a technical exchange and integration workshop is being planned for late summer of 2010 between the ASCEM and NRAP programs. The commonality of geologic models and flow and transport codes makes this area rich in collaborative potential.

- The DOE NNSA's ASC Initiative has invested heavily over the last 10 years in developing HPC capabilities. The ASCEM project is using former ASC personnel, leveraging existing experience on uncertainty quantification (UQ), verification and validation, model development, and large-scale simulation.

- The ASCEM team is also working with the Russian Academy of Sciences to evaluate alternative conceptual models for non-classical transport behavior in the vadose zone and looking for additional opportunities to collaborate internationally on HPC modeling and new programming models for the emerging multi-core computer architectures.

ASCEM will also maintain close ties with users through a User Steering Committee, LFRG, and the PA CoP. LFRG and PA CoP are both jointly sponsored by Offices in EM-30 and EM-40 and include participants/representatives from other DOE Offices and DOE contractors, National Laboratories, regulators, universities, and other user groups. ASCEM team members will provide briefings to both groups on a regular basis. The groups will also continue to be used to solicit representative user feedback and suggestions regarding ASCEM plans and activities.

LFRG is an independent group jointly chaired by representatives from EM-30 and EM-40 to verify, through review, that DOE, including the NNSA radioactive waste disposal facilities, protect the public and environment. It supports the implementation of DOE's regulatory responsibility under the Atomic Energy Act of 1954 (as amended) and DOE Order 435.1, *Radioactive Waste Management*. LFRG establishes teams to review performance assessments conducted for DOE disposal facilities and makes recommendations to DOE senior management regarding approval of the PAs and issuance of disposal authorizations. LFRG also serves as a forum for sharing experiences and lessons learned. Through it, participants provide a broad perspective and experience on complex-wide and site-specific issues related to radioactive waste management.

EM-30 and EM-40 jointly established PA CoP to enhance consistency in the preparation of PAs across the DOE complex, to foster the exchange of information among PA practitioners, and to develop appropriate guidance to ensure that PAs are based on sound science and thereby defensible. PA CoP is an open, user-oriented group, and the first two annual technical exchanges hosted by PA CoP have involved participants from multiple DOE HQ and Field Offices, national laboratories, contractors, universities, regulators, and international organizations involved in performance and risk assessment activities around the DOE Complex. PA CoP provides a central forum through which ASCEM gains access to a variety of potential users with practical perspectives regarding PA implementation and review.

The ASCEM User Steering Committee will solicit input from a cross-section of regulators (State, Environmental Protection Agency, Nuclear Regulatory Commission), oversight personnel (DOE HQ and Field Offices), and DOE contractors. The User Steering Committee will provide input directly to the ASCEM management team regarding plans and on-going development efforts.

8. IMPLEMENTATION SCHEDULE

As discussed, there are three major ongoing research initiatives in OTID. These include ASCEM, CBP, and GW&S. Below is a description of the effective integration of these three research initiatives around ASCEM's central transformational efforts. The technical impacts from the Landfill Partnership will be incorporated into the CBP source term modules that will be supplied to ASCEM. Key to the integration of these programs is the establishment of near- and long-term hard and soft integration points. The window of integration is between FY11 and FY14 in order to fully deploy the new ASCEM tool by FY14. This section describes the Integration Plan as shown in *Figure 7*.

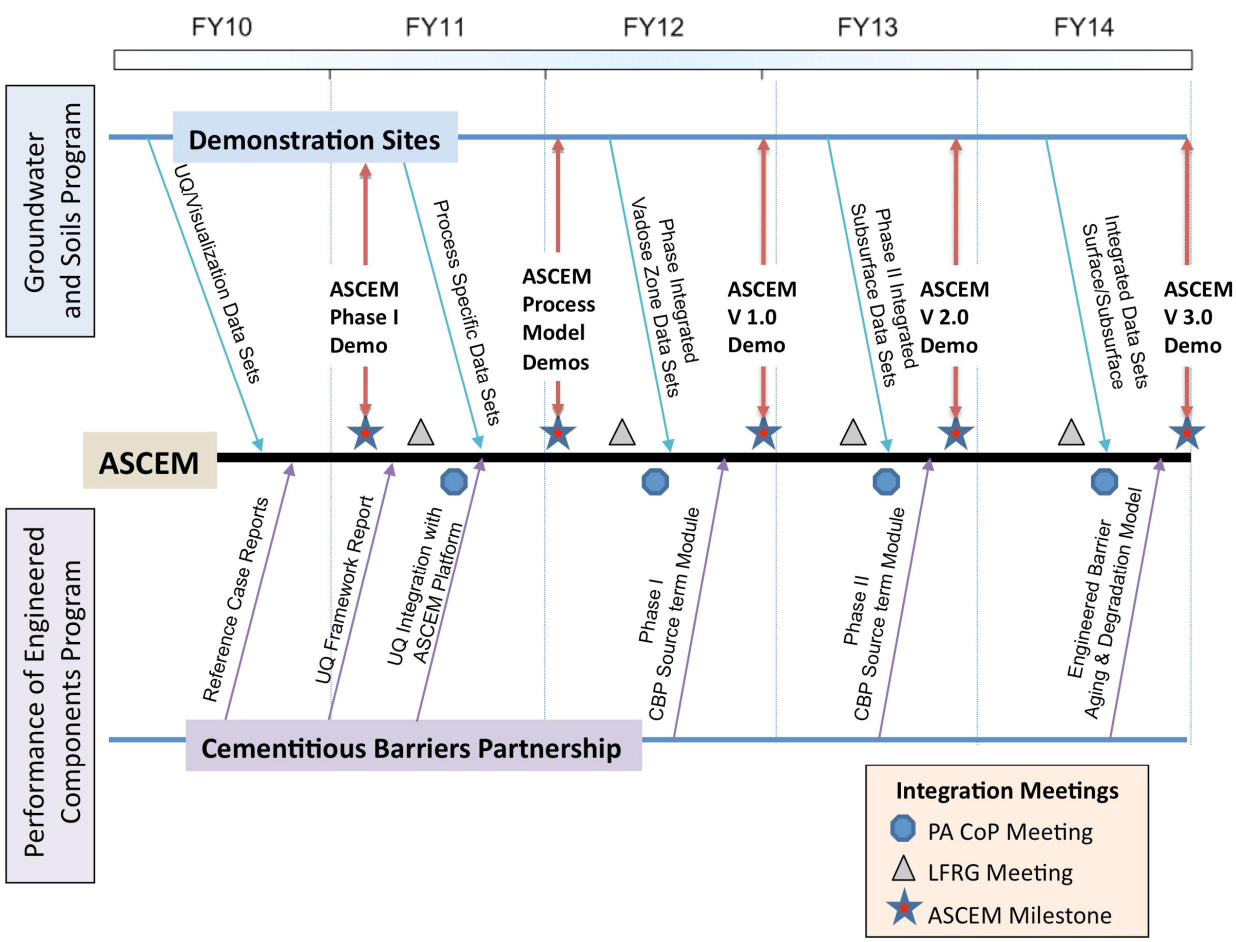

Figure 7. Schematic example of integration plan for ASCEM, CBP and EM-32 GW&S field site demonstrations.

There are three research sites in the GW&S area. Information from these sites will be used to demonstrate and validate the ASCEM platform and HPC core. The ASCEM demonstration and validation sites will be chosen from the draft sites end-user needs report [2] and will offer superior opportunities to test and refine the ASCEM codes.

9. INTEGRATED MODELING WBS AND MILESTONES

ASCEM's work scope uses a standard work breakdown structure (WBS) as the basic building block for planning all authorized work. The WBS forms the structure for integration and management of the project scope, schedule, and budget. Although not illustrated below, the ASCEM WBS structure is integrated within the OTID WBS. *Figure 8* shows the project WBS-defined to the third level, and illustrates ASCEM relationships, interfaces, dependencies, and ties to the OBS shown in *Figure 5*.

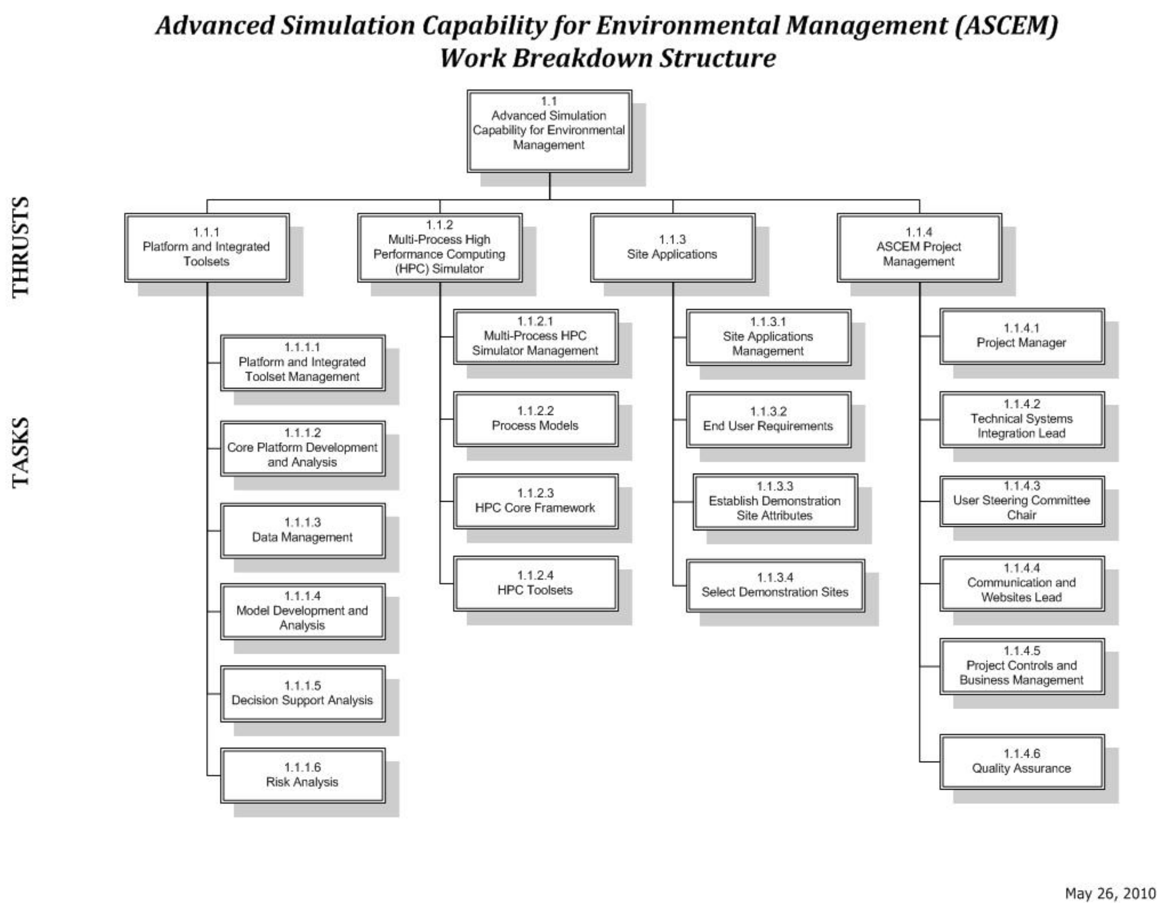

Figure 8. WBS elements of the ASCEM program.

The following section describes the goals and deliverables for the ASCEM Program over the next 4 years. The goals set high-level expectations for ASCEM's accomplishments each year. The deliverables are specific documents or decision points that the ASCEM multi-laboratory team will be held accountable for each year. The deliverables are also highlighted in the attached ASCEM P6 project plan.

9.1. Integrated Goals and Deliverables

FY11

- Use ASCEM Version 1.0 to conduct simulations in support of the development and demonstration of innovative strategies and *in-situ* technologies that attenuate and achieve sustainable immobilization in subsurface environments to eliminate contaminant fluxes to water resources.

- Use ASCEM Version 1.0 to conduct simulations in support of the development and demonstration of minimally invasive access and delivery methods to emplace remediation amendments in deep vadose zone environments.

- Use ASCEM Version 1.0 to develop and demonstrate advanced characterization technologies (e.g., geophysical technologies) to assess contaminant spatial distributions and hydrological connections between water resources (e.g., groundwater, karst system, and surface water), and to provide continuous oversight of plume behavior and support remedy emplacement, optimization, and performance monitoring.

- Use ASCEM to develop and demonstrate innovative approaches to measure, predict, and monitor the long-term impacts of remedial strategies in deep vadose zone environments.

- Use ASCEM to maximize the understanding of subsurface heterogeneities to minimize sampling and analysis costs, improve remediation amendment emplacement, and develop *in situ* and geophysical measurement techniques for key parameters *(collaboration with DOE-SC).*

- Use ASCEM Version 1.0 to improve the understanding of biochemical and environmental controls on mercury speciation and food chain transfer *(collaboration with DOE-SC).*

- *CBP Schedule Tie*: Complete CBP UQ framework report and provide to ASCEM.

- *CBP Schedule Tie*: Develop initial one-layer diffusion model for species ingress and release from a cement monolith (*necessary for CBP Phase I Module*).

- *Landfill Partnership Schedule Tie:* Prepare first year reports from applied research projects and provide to ASCEM.

FY12

- Use ASCEM Version 1.0 to integrate new data and information from integrated field sites to iteratively evaluate the alternative approaches for treating key contaminants.

- *CBP Schedule Tie*: Develop prototype CBP Phase I Module and provide to ASCEM.

- *CBP Schedule Tie*: Include damage mechanics for sulfate attack in thermodynamic model for cement pastes, mortars and concrete (*necessary for Phase I Module*).

- *CBP Schedule Tie*: Develop multi-layer diffusion model for two or more layers of dissimilar materials (e.g., grout, concrete, soil).

- *CBP Schedule Tie*: Evaluate effects of various levels of cracking on one- and multi-layer CBP models.

FY13

- Use ASCEM Version 2.0 to conduct simulations in support of the development and demonstration of innovative strategies and *in-situ* technologies that attenuate and achieve sustainable immobilization in subsurface environments to eliminate contaminant fluxes to water resources.

- Use ASCEM Version 2.0 to conduct simulations in support of the development and demonstration of minimally invasive access and delivery methods to emplace remedial amendments in deep vadose zone environments.

- Use ASCEM Version 2.0 to conduct simulations to support development and demonstration of advanced characterization technologies (e.g., geophysical technologies) to assess contaminant spatial distributions and hydrological connections between water resources (e.g., groundwater, karst system, and surface water), and to provide continuous oversight of plume behavior, support remedy emplacement, optimization, and performance monitoring.

- Use ASCEM Version 2.0 to conduct simulations in support of the development and demonstration of innovative approaches to measure, predict, and monitor the long-term impacts of remediation strategies in deep vadose zone environments.

- Use ASCEM Version 2.0 to conduct simulations to maximize the understanding of subsurface heterogeneities to minimize sampling and analysis costs, improve remedial amendment emplacement, and develop *in situ* and geophysical measurement techniques for key parameters *(collaboration with DOE-SC)*.

- Use ASCEM Version 2.0 to conduct simulations to improve the understanding of biochemical and environmental controls on mercury speciation and food chain transfer *(collaboration with DOE-SC)*.

- *CBP Schedule Tie*: Develop CBP Phase II Module and provide to ASCEM.

- *CBP Schedule Tie*: Develop scenario model for tank closure, cementitious waste form in concrete vault, and *in situ* grouting of soil contaminants.

FY14

- Use ASCEM Version 2.0 to integrate new data and information from integrated field sites to iteratively evaluate the alternative approaches for treating key contaminants.

- *CBP Schedule Tie*: Develop scenario model for facility entombment.

FY15

- Use ASCEM Version 3.0 to integrate new data and information from integrated field sites to iteratively evaluate the alternative approaches for treating key contaminants.

FY16

- Use ASCEM Version 3.0 to integrate new data and information from integrated field sites to iteratively evaluate the alternative approaches for treating key contaminants.

10. ASCEM INTEGRATED IMPLEMENTATION SCHEDULE

P-6 schedule under development

10.1 Budget

The *baseline budget* is formed by the cost estimates and assumptions that support execution of the baseline scope and schedule, as resource-loaded onto the detailed baseline schedule. Resources (such as labor, travel, procurements, and subcontracts) are estimated for each detailed schedule activity at each laboratory to provide the budget basis for the work to be performed in each thrust area. The cost estimates for each detailed schedule activity provide the basis for thrust area, task, and total project time-phased cost estimates.

11. PROJECT PERFORMANCE AND MONITORING (Risk and Contingency Plans)

A Risk Management Plan provides guidance for identifying and mitigating the technological and human risks associated with developing and deploying ASCEM.

Risk is defined here as: **Risk R = *likelihood of occurrence * consequences of failure***

Neither the likelihood of occurrence nor the consequences of failure have numerical values to support any ASCEM risk management task. All ASCEM risk management will be addressed qualitatively. The principles of ASCEM risk management are described in the ASCEM Baseline Management document [3].

The mechanism to track and report risks is the monthly earned value management report (EVMS). In this report, the ASCEM Program Manager, Technical Integration Lead, and the Thrust Leads have the responsibility to document monthly cost and schedule progress, as well as identify and develop mitigation plans for all their identified risks. Through the Monthly EVMS report, the ASCEM Multi-Lab Program Manager reports these risk mitigation plans to DOE-EM for their concurrence. If the mitigation strategy appears to be ineffective, the Project Manager and Thrust Leads should discuss other options and engage DOE-EM and subject matter experts who might aid the risk reduction effort.

In addition to the standard EVMS tools described above to monitor progress of the ASCEM program, project technical direction will be monitored through peer review. Peer reviews of Federal technical programs have recognized value within government agencies [9, 10, 11]. Selected, independent subject matter experts will review key planning documents and deliverables. Review findings and recommendations will be used to ensure the creation of high quality products and to improve end user acceptance. Upon DOE request, the Multi-lab ASCEM Management and Integration Team will provide technical support to the reviews.

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APPENDIX A - ACRONYMS AND ABBREVIATIONS

ASC	Accelerated Strategic Computing
ASCEM	Advanced Simulation Capability for Environmental Management
BPASSP	Biogeochemical Processes for the Applied Subsurface Research Program
CBP	Cementitious Barriers Partnership
CoP	Community of Practice
CRESP	Consortium for Risk Evaluation with Stakeholder Participation
D&D	Decontamination and Decommissioning
DOE	Department of Energy
DVZAP	Deep Vadose Zone Applied Research Program
EM	Office of Environmental Management
EPA	Environmental Protection Agency
EVMS	Earned Value Management Report
FE	Office of Fossil Energy
GW&S	Groundwater & Soil Remediation Program
HPC	High Performance Computing
LFRG	Low-Level Waste Disposal Facility Federal Review Group
NAS	National Academy of Sciences
NE	DOE Office of Nuclear Energy
NNSA	National Nuclear Security Administration
NRAP	National Risk Assessment Program
NRC	National Research Council
NSC	National Security Complex
OBS	Organizational breakdown structure
ORNL	Oak Ridge National Laboratory
ORR	Oak Ridge Reservation
OTID	Office of Technology Innovation and Deployment
PA	Performance Assessment
PA CoP	Performance Assessment Community of Practice
QA	Quality Assurance
RCRA	Resource Conservation and Recovery Act
R&D	Research and development
SBR	Subsurface Biogeochemical Research Program
SC	Office of Science (DOE)
SciDAC	Scientific Discovery through Advanced Computing
SFA	Science Focus Area
SRNL	Savannah River National Laboratory
SRS	Savannah River Site
UQ	Uncertainty Quantification
WBS	Work Breakdown Structure

APPENDIX B - Cementitious Barriers Partnership (CBP)

CBP is a collaborative program sponsored by the DOE Office of Waste Processing. The objective of the CBP is to develop a set of computational tools to improve understanding and prediction of the long-term structural, hydraulic, and chemical performance of cementitious barriers and waste forms used in nuclear applications. CBP tools will reduce the uncertainties of current methodologies for assessing cementitious barrier performance and increase the consistency and transparency of the assessment process.

The CBP is composed of CRESP/Vanderbilt University, Energy Research Centre of the Netherlands, the National Institute of Standards and Technology, SRNL, SIMCO Technologies Inc., U.S. Nuclear Regulatory Commission, and DOE-EM. The partnership is administered through a Cooperative Research and Development Agreement (WSRC CRADA No. CR-08-001), an Interagency Agreement, and a Memorandum of Understanding. Funding comes from DOE-EM and CRESP.

Objectives

The CBP project is a five-year effort to reduce uncertainties in current methodologies for assessing cementitious barrier performance and increasing the consistency and transparency of the assessment process. This effort will further support several of the strategic initiatives in the DOE Office of Environmental Management Engineering and Technology Roadmap, including the following:

1) Enhanced tank closure
2) Enhanced stabilization technologies
3) Advanced predictive capabilities
4) Enhanced remediation methods
5) Adapted technologies for site-specific and complex-wide D&D applications
6) Improved SNF storage, stabilization, and disposal preparation
7) Enhanced storage, monitoring, and stabilization systems
8) Enhanced long-term performance evaluation and monitoring.

A credible set of simulation and modeling tools will be developed to predict the structural, hydraulic, and chemical performance of cement barriers used in nuclear applications over extended time frames (e.g., up to or longer than 100 years for operating facilities and longer than 1000 years for waste management). The results will enable improved, risk-informed, performance-based decision-making and will be applicable to Hanford and SRS closure activities as well as other DOE sites and future nuclear facilities (leveraging work done by the Nuclear Regulatory Commission and DOE-NE).

Approach

CBP research consists of 1) improving conceptual and computational models for the durability of cementitious materials and waste forms, 2) conceptual model verification through laboratory experiments and analysis of field specimens, and 3) model parameterization using simulated and actual sample characterization. These efforts will form the basis for improved modeling and simulation tools and techniques to quantify and reduce the uncertainty associated with assessments.

Reference cases have been defined to provide a common set of system configurations to illustrate and evaluate CBP methods and tools. Reference cases include 1) a cementitious low activity waste form in a reinforced concrete disposal vault, 2) a closed high-level waste tank, and 3) a spent nuclear fuel basin during operation. Additional cases of grouting and entombment of a canyon building and *in situ* grouting of vadose contamination are under development based on requests from DOE-RL.

Modeling will be based on the evolution, coupling, and integration of new and existing models and parameter measurement techniques. Existing models will be improved and new models developed in conjunction with an integrated experimental program to 1) reduce important uncertainties, 2) measure needed model parameters, and 3) validate and quantify uncertainties for the integrated models. A modular approach will be used to develop the integrated tools to predict the hydraulic properties and stability of radionuclides and cement matrix phases and release fluxes of constituents. The level of engineering detail needed to use CBP tools will be flexible and based on the requirements of the analyses.

CBP produced a series of reports describing the following:

- The QA program (CBP-01)
- A review of PA and PA-like assessments (CBP-TR-2009-001)
- State-of-the-art reviews of the performance of cementitious barriers used in radioactive waste treatment and disposal (CBP-TR-2009-002)
- Descriptions of the component codes and integration platform selected for CBP (CBP-TR-2009-003).

These reports are available at www.cementbarriers.org.

Relevance and Impact to DOE

Evaluations of historic PAs show that engineered barriers are needed to prevent radionuclide release into the environment from near-surface nuclear facilities. In the absence of adequate predictive tools, assessments cannot fully incorporate the effectiveness of cement barriers used in containment and/or as part of the waste zone. This limits both the inventory of radionuclides that may be safely disposed of in shallow land disposal and the predicted service life of operating nuclear facilities. The efficacy of cementitious materials as barriers to the release of contaminants affects all disposal sites that use cementitious waste forms and concrete and grout structures, those that perform D&D activities and service life determination of existing structures, as well as the design of future public and private nuclear facilities. CBP tools are also applicable to closure of major facilities (e.g., canyons and basins), *in situ* immobilization of contaminated vadose zone materials, and the storage of these materials at new nuclear facilities. CBP efforts will enable improved, risk-informed, performance-based decision-making for the next generation of commercial nuclear reactor waste disposal sites.

One significant benefit to DOE is the collaborative effort and information exchange among CBP partners resulting in early identification and resolution of key technical issues and uncertainties, improved transparency and credibility, and acceptance of the methodologies adopted by DOE. Additional benefits include:

- More efficient use of materials and improved designs
- Reduced uncertainty from improved conceptual models, computational models, and data
- Shorter analysis time due to integration of simulation components
- Shorter review time and clearer stakeholder interactions because of improved transparency
- Reduced potential for human error through the integration of process steps.

Finally, CBP processes and organizational characteristics may well also serve as a model for similar evaluation of other waste form and/or barrier materials.

Relationship to ASCEM

CBP software tools will offer a specialized capability to predict physical and chemical properties of cementitious materials through time and space, and the transport/leaching of contaminant species from cementitious waste forms and through concrete barriers. CBP is focused on phenomena occurring in the near-field, within and adjoining engineered structures and contaminant source zones, at the centimeter to meter scale, with supporting materials characterization provided at smaller scales as necessary. The software modules developed by CBP will become modules within the ASCEM system model for source zone material properties and/or contaminant flux.

Major CBP Reports (see www.cementbarriers.org)

CBP 2009a, *Description of the Software and Integrating Platform* (Contains Four Chapters), CBP-TR-2009-003, Rev. 0, Cementitious Barriers Partnership, Aiken, SC and Nashville, TN. Available from: http://cementbarriers.org/reports.html.

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APPENDIX C - DOE Landfill Partnership

At most sites in the DOE complex, decommissioning is contingent on the availability of an on-site disposal facility. Thus, the ability to efficiently and cost effectively design and construct on-site disposal facilities significantly impacts the cost and schedule of decommissioning projects. This is complicated by the notorious difficulty in achieving stakeholder buy-in for a facility meant to contain on-site wastes in perpetuity. Stakeholder buy-in is also affected by contrasting and/or conflicting technical requirements in government regulations (e.g., the U.S. Environmental Protection Agency's [EPA's] Resource Conservation and Recovery Act vs. DOE's 435.1) as well as insufficient stakeholder confidence in containment systems, PAs, and monitoring systems. The purpose of the DOE Landfill Partnership, supported by EM-30, is to conduct the applied research and to facilitate the technical dialogue needed to build confidence in technologies used for on-site disposal facilities, the methodology used to design facilities, the modeling strategies used for PAs, and the systems used to monitor long-term performance.

Objectives

The DOE Landfill Partnership has two primary objectives:

(1) To address technological issues related to on-site disposal facilities ("landfills") in the DOE complex that receive low-level wastes and mixed wastes from decommissioning projects, including design, operations, and predicting long-term performance

(2) To facilitate dialogue between key stakeholders influencing design and monitoring of disposal facilities (e.g., EPA, U.S. Nuclear Regulatory Commission, DOE, and state agencies). The technical objective is focused on developing technical solutions, modeling strategies, and data that build confidence in DOE disposal operations while also resulting in lower costs, more expedient construction or operations, improved performance (in the context of DOE regulatory requirements), and more effective monitoring. The stakeholder objective is intended to resolve contrasting and/or contradictory regulatory issues that impede facility design and performance, with the ultimate goal of creating a harmonious regulatory structure for disposal facilities.

Approach

A series of independent technical reviews conducted in FY07 and FY08 and a DOE landfill workshop held in FY09 identified several themes requiring technological development for on-site disposal facilities. These reviews also revealed technical inconsistencies in state and federal regulations regarding disposal facilities, identified deficiencies in predictive capabilities, and illustrated that the approval of on-site disposal facilities was impeded significantly by resolution of deficiencies and inconsistencies. The DOE Landfill Partnership was initiated in FY10 as a vehicle to address these technological and regulatory challenges.

The partnership consists of a technical working group composed of members from the CRESP and DOE, along with key regulatory stakeholders from EPA, U.S. Nuclear Regulatory Commission, DOE and personnel from Washington, Utah, South Carolina, Tennessee, Texas and Ohio state agencies. This group of partners 1) identifies applied research activities necessary to resolve technical issues and build stakeholder confidence and 2) develops/recommends approaches to remedy inconsistencies and contradictions in existing regulations. Topics in the applied research agenda for FY10-11 include radionuclide transport in barrier systems, innovative methods for waste characterization/forecasting, and evolutionary final cover designs.

Relevance and Impact to DOE

Throughout the DOE complex, decommissioning and remediation as well as other waste management activities are contingent on the availability of on-site disposal facilities. Thus, the ability to design and construct on-site disposal facilities in a cost-effective and expedient manner significantly impacts the cost and schedule of decommissioning projects. These factors are complicated by the notorious difficulty in achieving stakeholder acceptance for a facility meant to contain wastes on-site, essentially in perpetuity. The Landfill Partnership will apply its expertise at DOE sites like Hanford where decisions on whether to cap/solidify in-place or to excavate/transfer waste to landfills will be central to a wide variety of major decisions in the Central Plateau and the River Corridor. At Hanford, these landfill-related decisions must be closely coordinated with continuing work (e.g., with CBP) to define the efficacy and durability of waste forms and waste placement/containment scenarios (e.g., trenches) where waste forms are placed/stored prior to final disposition in landfills. To this end, the Landfill Partnership is designed to help ensure consistent and efficient coordination across multiple organizations.

Relationship to ASCEM

The DOE Landfill Partnership will provide input on modeling the performance of landfill disposal systems with emphasis on the performance of landfill caps and liners under expected DOE management conditions at selected sites (e.g., Hanford, Idaho, Savannah River, and Oak Ridge). The Landfill Partnership will generally focus on near-field phenomena that influence the release and transport of contaminants from various landfill configurations, which is of particular concern to the ASCEM initiative.

APPENDIX D – Integrated Strategy at 3 Field Research Sites

Biogeochemical Processes for Applied Subsurface Science Program at Savannah River

Attenuation of metals and radionuclides is integral to achieving remediation objectives for contaminated groundwater. Metals and long-lived radionuclides, those posing the greatest risk to the environment, typically are not destroyed during treatment, leading to either in-place treatment or removal followed by treatment. Pump-and-treat approaches employing *ex situ* (above ground) treatment methods are not economically feasible and in many instances will create additional waste streams requiring further treatment. For in-place treatments to be successful, the contaminants must be stabilized or detoxified for periods of time that are on the order of hundreds to thousands of years. An inherent truth is that once the source of contamination is removed, in time, all waste sites will evolve to their natural condition. Thus, the metal and radionuclide contaminants must be stable or non-toxic in the setting. Success is predicated on understanding the attenuation mechanisms and their effects on contaminant mobility. Technical issues associated with this understanding are:

- Addressing heterogeneity in hydrogeological and geochemical properties within aquifers
- Understanding how small-scale field and laboratory measurements relate to field-scale processes
- Accounting for adsorption of contaminants.

These issues have been studied extensively, but the research has not crystallized into application-based approaches that are readily employed at many waste sites or approaches that are tractable for the average waste site owners.

To develop an applied science solution resulting in "tools" that are transferable to the DOE Complex, the Biogeochemical Processes for the Applied Subsurface Research Program (BPASSP) at the SRS will integrate the following information:

- End-users' experience with site history, operational constraints, and budgetary issues
- SC's wealth of basic science knowledge
- Regulator expectations to ensure consistency with regulatory policy and guidance.

In addition to the information represented above, BPASSP will provide ASCEM with data on site-specific hydrogeology and biogeochemistry, defining contaminant source and plume characteristics and controlling processes, and on remediation strategies, including remediation and monitoring technology implementation and performance metrics. Together, this information will help ASCEM transition its scientific results into "tools" applicable first at the Savannah River Site, and then transferable across the entire DOE complex.

Deep Vadose Zone-Groundwater Applied Research Program at the Hanford Site

Controlling the source of contamination is integral to meeting remediation objectives for mitigating direct exposure to contamination and limiting the flux of contamination to groundwater.

Functionally, the methods for addressing subsurface contamination must remove contamination and/or reduce the transport of contaminants through the vadose zone. However, this problem is particularly challenging in vadose zone environments, which consist of complex stratified layers of unconsolidated and water-unsaturated sediments that are, in many places, contaminated with radionuclides, metals, organics, and, in some cases, complex mixtures. They serve as a potential source of groundwater contamination and as the primary conduit for transport from the ground surface. If contamination is in the deep vadose zone and disperses to the associated groundwater, *in situ* remediation technologies or defensible technical data and justification for enhanced attenuation may be the only ways to perform effective remediation. These technologies may provide the only viable paths to long-term stewardship of sites contaminated with metals and long-lived radionuclides other than costly, ineffective, and impractical physical removal techniques.

Systematic gaps in the technical foundation supporting environmental decisions have led to ineffective remediation and uncoordinated policies [6]. Lack of understanding of key processes (e.g., biogeochemical and hydrologic) affecting contaminant migration makes it difficult to predict the location, transport, and fate of these contaminants in the subsurface. These factors also make it difficult to design and deploy sustainable remediation approaches and monitor the long-term behavior of remediation actions. As highlighted by the National Academy of Science [7, 8], for DOE-EM to successfully address remaining cleanup problems, it will require 1) partnering and leveraging with other relevant organizations, and 2) integrating basic science and "needs driven" applied research activities with DOE-EM cleanup operations to facilitate the transition of scientific results into applied solutions.

The Deep Vadose Zone Applied Research Program (DVZAP) and ASCEM are two of the tools that will aid DOE-EM in transitioning scientific results into applied solutions. The DVZAP will provide ASCEM with information on site-specific hydrogeology and biogeochemistry defining contaminant source characteristics and controlling processes. It will also provide information on remediation strategies, including remediation and monitoring technology implementation and performance metrics. ASCEM will use this information to assess the performance of remediation strategies and, through integration with the DVZAP, facilitate development of the scientific foundation, applied technologies, and remediation strategies necessary to make sound and defensible remediation decisions that will successfully meet the target cleanup goals in a manner that is acceptable to regulators.

Mercury Remediation and Characterization Program at Oak Ridge

Historic uses of mercury at the Oak Ridge Reservation in Oak Ridge, TN, have resulted in contamination at the Y-12 National Security Complex (NSC) and Oak Ridge National Laboratory (ORNL). East Fork Poplar Creek, for example, has been posted with a fish consumption advisory as a result of mercury contamination. Remediation actions at Y-12 have reduced mercury inputs to the creek by more than 90%, but stream water and fish remain impacted. Additionally, D&D activities at Oak Ridge are expected to result in physical disturbances that may release additional mercury to soil, groundwater, and surface water. Development of *in situ* remediation and characterization technologies and a systems approach to assessing contaminant fate and transport is a key strategy for attaining regulatory compliance during D&D and long-term stewardship of sites contaminated with mercury. Approaches developed to address mercury can be adapted for use with other metals, radionuclides, and organic contaminants.

ORNL and Savannah River National Laboratory (SRNL) lead EM's mercury remediation and characterization program. This program is tasked with developing cost-effective technical solutions for waterborne mercury remediation, soil treatment, source zone identification, mercury characterization, and conceptual and numerical modeling of contaminant fate and transport. Waterborne mercury is addressed through the development and demonstration of innovative methods that use specialized resins, unique nanomaterials, or chemical addition to transform, absorb, and/or remove mercury. Soil treatment targets *in situ* and *ex situ* approaches for removing mercury or stabilizing it within environmental matrices. Source-zone identification and characterization focuses on developing and deploying analytical tools and sampling approaches that can be used for *in situ*, real-time identification of mercury concentrations and speciation in soil, soil gas, and water. Finally, conceptual modeling is being used to identify site-specific mercury transport pathways, expected transformations, and fluxes, information that in turn guides numerical models that account in detail for speciation reactions, biogeochemical conditions, and site hydrogeology. Integrated characterization, remediation, and modeling efforts will improve the ability to predict mercury releases and transport, prevent new contamination, identify and characterize existing contamination, remediate impacted zones, and reduce cost, uncertainty, and risk at DOE sites. Applied research is performed in collaboration with the ORNL Science Focus Area (SFA) program, DOE's Oak Ridge Operations Office, and the Babcock & Wilcox Y-12 NSC contractor.